Trace Gas Re-Processing Activities at NOAA/NESDIS

Chris Barnet & Mitch Goldberg
NOAA/NESDIS/STAR

Mar. 8, 2006
AIRS Science Team Meeting

Walter Wolf: Near Real Time Processing & Gridding System
Lihang Zhou: Regression Retrieval & Near Real Time Web Page
Eric Maddy: CO_2 retrieval, tuning, vertical averaging functions.
Xiaozhen Xiong: CH_4 retrieval
Xingpin Liu: Re-processing, Statistics, Trace gas web-page
Fengying Sun: New RTA upgrade installation & checkout
Jennifer Wei: START experiment laison & O_3 retrieval
Murty Divakarla: Operational sonde database (T(p) & q(p) biases)

Topics

- PGE Issues with regard to trace gases
- SO_2 flag and Product Development
- Reprocessing of NOAA/NESDIS gridded products.
- CH_4 Product & Validation Efforts
- CO_2 Product & Validation Efforts

Retrieval of Atmospheric Trace Gases Requires Unprecedented Instrument Specifications

- **Need Large Spectral Coverage (multiple bands) & High Sampling**
  - Increases the number of unique pieces of information
    - Ability to remove cloud and aerosol effects.
    - Allow simultaneous retrievals of T(p), q(p), O_3(p).
- **Need High Spectral Resolution & Spectral Purity**
  - Ability to isolate spectral features → vertical resolution
  - Ability to minimize sensitivity to interference signals..
- **Need Excellent Instrument Noise & Instrument Stability**
  - Low NEΔT is required.
  - Minimal systematic effects (scan angle polarization, day/night orbital effects, etc.)

PGE Issues with regard to Trace Gases

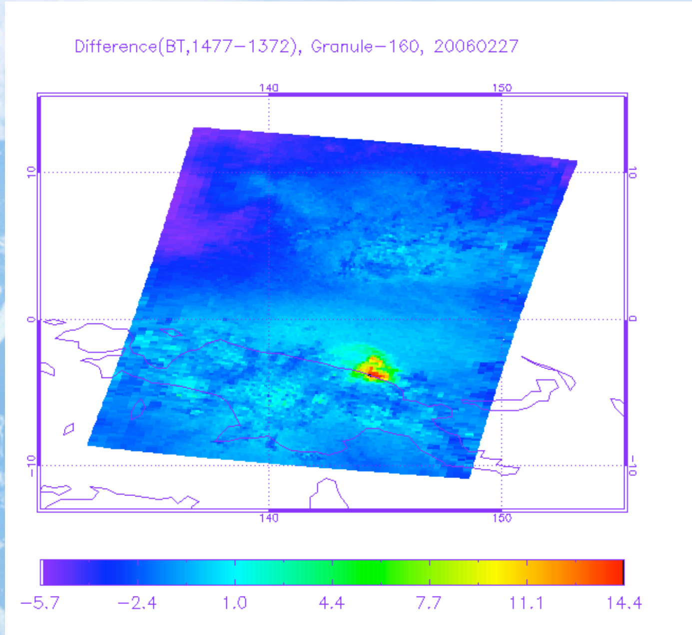
- New RTA "wrapper" delivered to GSFC in early Dec. 2005 for incorporation into PGE.
- We accomplished closure on tuning w.r.t. coordinated sondes
  - Mixed use of retrieval and sonde products to compute a tuning in which LW & SW agree and radiance tuning is minimized
  - Major impact for trace gas retrievals.
- Datasets for microwave tuning delivered to MIT in late Dec. 2005.
- A number of CO_2 climatologies explored: Simple CO_2 climatology installed for v5.0 at JPL.
- Vertical averaging *estimate* is ready to install into PGE v5.0. Improvements to averaging function anticipated for future PGE upgrades. Suggest Eric Maddy work directly with John Blaisdell and/or Evan Manning to install into PGE.

PGE Issues with regard to Trace Gases

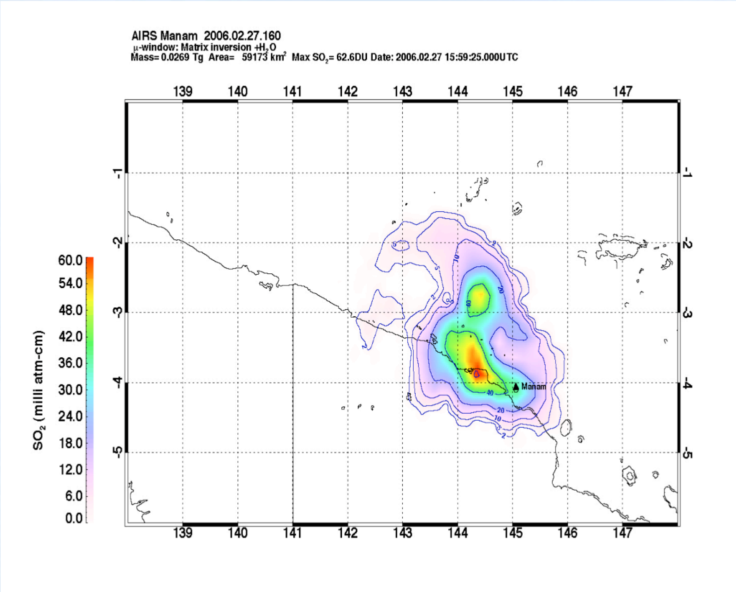
- Ad-hoc model error term has been removed for v5.0
- (Sep. 2005) Recommended that we use information content and residual's in rejection criteria – we added this to NOAA QA of trace gas products.
- Add physical error co-variance terms
  - CO2 in T(p) and cloud clearing (installed in PGE)
  - CH4 in q(p): negligible impact, unless we want to use CH4 channels in q(p) retrieval - I suggest we ignore this for now.
  - HNO3 in surface and CH4 and q(p): not needed unless we use HNO3 channels in q(p) and surface retrieval
  - P_{surf} error in T(p) and q(p) retrievals: TBD (post v5 ?)
- Ozone Regression – attempt at new training
  - Needs more work – not ready for v5.0

SO2 flag has generated a lot of interest at NOAA and internationally

- Augustine (1/13,14,29/06, 2/7/06) & Manam (2/27-28/06) detected
- Washington Volcanic Ash Advisory Center (VAAC, W-vaac@noaa.gov) requested and now receives and re-broadcasts AIRS SO2 flag.
    - May be used for aircraft early warning.
- Fred Prata, Norwegian Institute for Air Research, is generating SO2 retrievals from AIRS & HIRS - we are working with Fred to incorporate his retrieval into the near real–time system



AIRS SO2 flag



SO2 Retrieval (Courtesy of Fred Prata

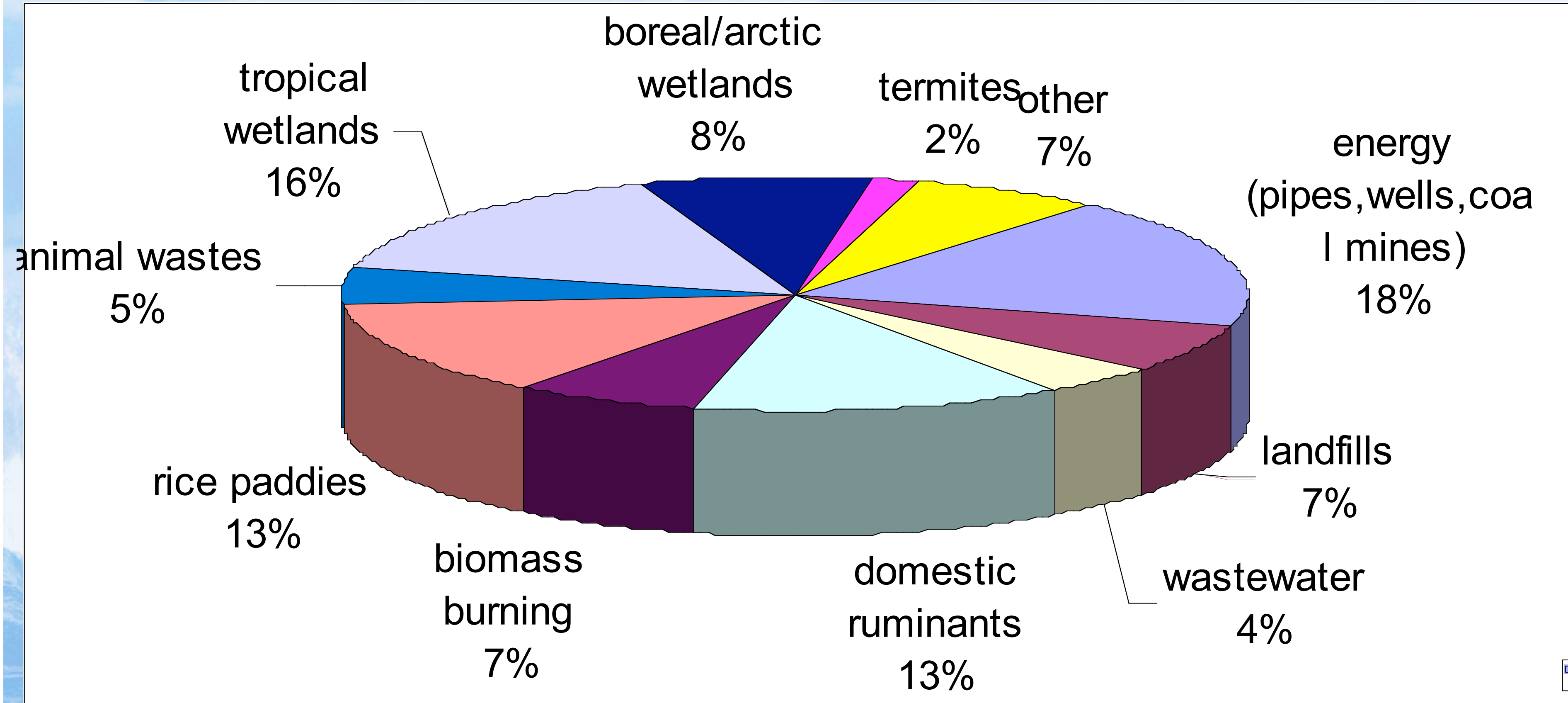
Re-processing using AIRS Golf-ball Subsets

- This activity utilizes the near real time AIRS processing system developed by Mitch Goldberg, Walter Wolf, and Lihang Zhou
- The complete AIRS golf-ball closest to the mid-point of a fixed 3^o x 3^o uniform grid is extracted and saved
  - 120 longitude by 61 latitude cells
  - Separate file for ascending and descending orbits
  - AIRS, AMSU, and HSB L1b
  - ECMWF, and GFS forecast files
  - MODIS L1b on AIRS FOV's available since 11/04 (clear & cloudy)
    - However, incorrect spatial footprint was used. Corrected Jan. 06
- $\approx$2x6500 =13,000 golf-balls saved per day since Aug. 2003
  - 13,000/324,000 = 1:25 of full-resolution data.
- Reprocessing Advantage
  - 2.5 years can be re-processed in a few days (on 8 generic cpu's)
  - Small systems (< 16 TB) can hold entire dataset
    - L1b radiances, ECMWF, AVN, and multiple sets of ret products.

Reprocessing of trace gas products

- Three runs emulating v4.0, v4.2 (new ε), v4.7 (new RTA & tuning) have been finished and analyzed.
  - Analysis and modifications to the retrieval system based on this analysis are being performed.
- A new run emulating a "v5.0" system will be started in a few weeks.
  - Result of this run will be provided to modelers with preliminary internal vertical averaging analysis.
- Web page display of products (see Sep. 27, 2005)
  - Has scientific value to locate interesting features.
  - Unfortunately our IT security issues at NOAA prevent outside user access at this time – we are trying to resolve this.

Methane Sources



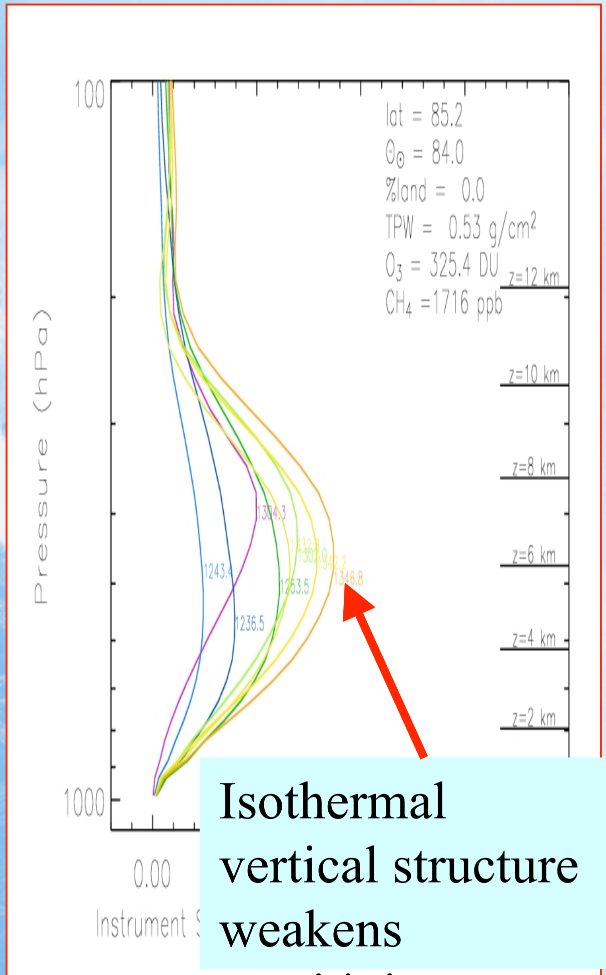
Ref.: Lelieveld, 1998 & Houwelling 2002 (600 Tg total)

Note: Approximately 50% of sources are anthropogenic

Trees (Keppler et al. 2005) may contribute 62-235 Tg (10-35%), mostly in tropics

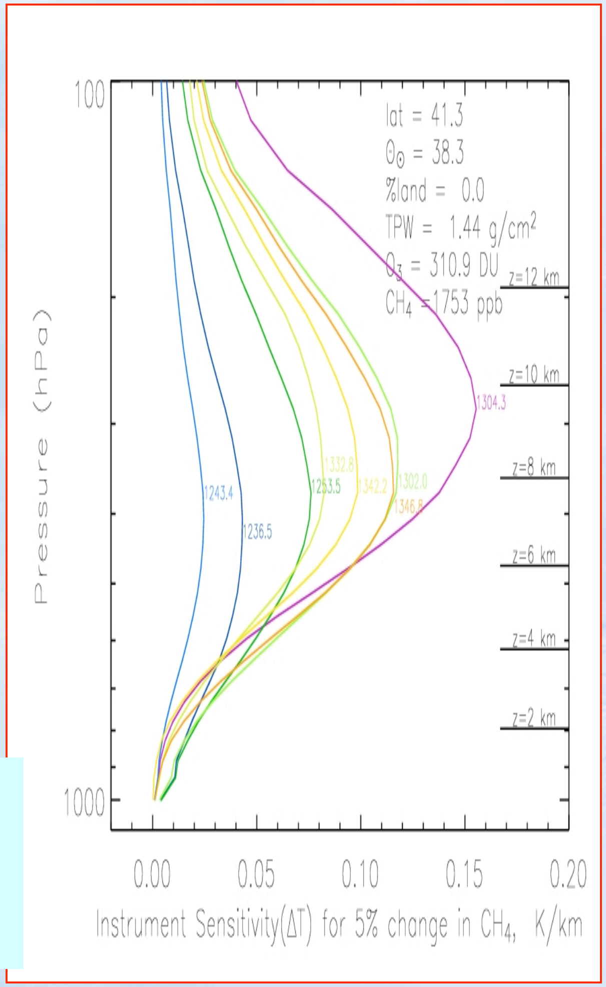
AIRS CH_4 Kernel Functions are Sensitive to $H_2O(p)$ & $T(p)$

Polar

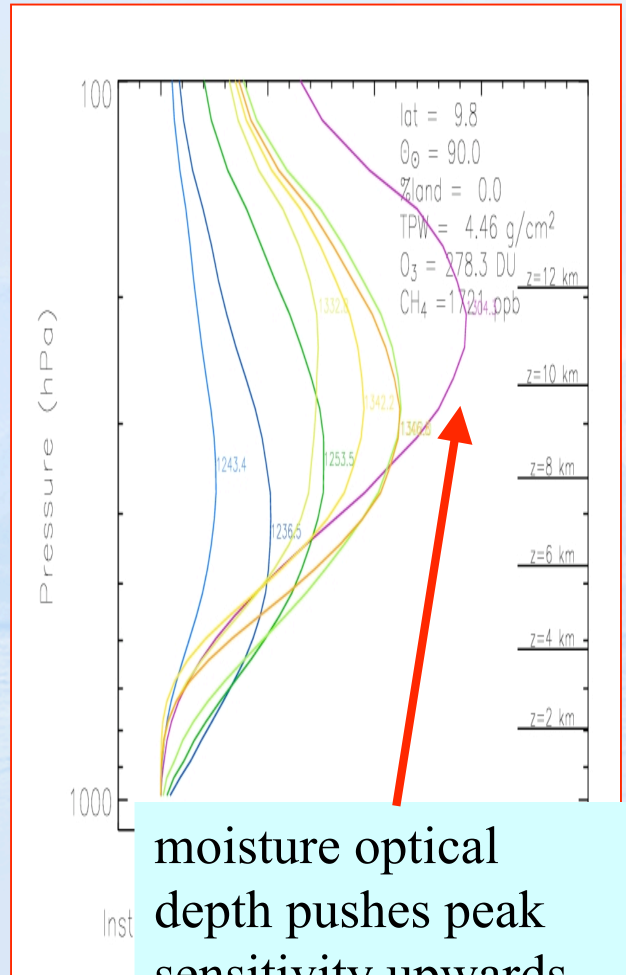


Isothermal vertical structure weakens sensitivity.

Mid-Latitude

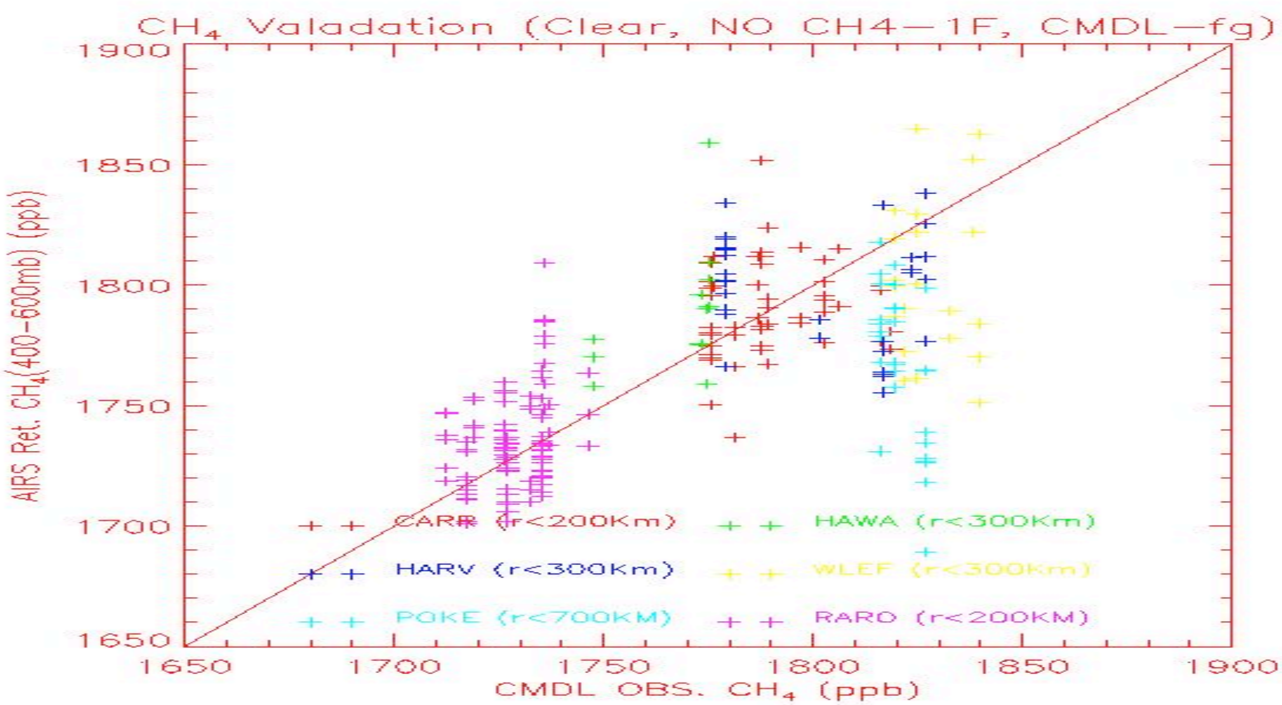


Tropical



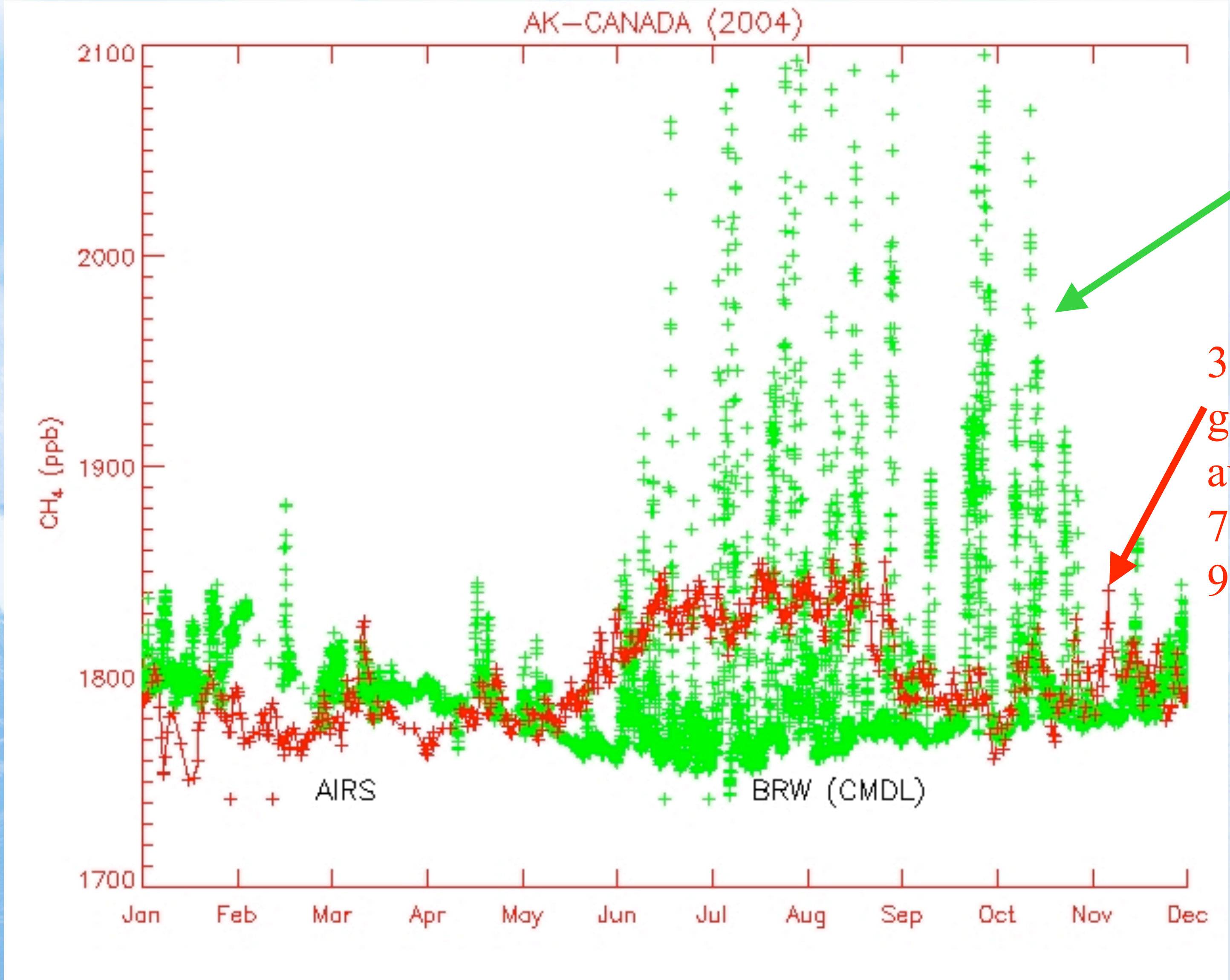
moisture optical depth pushes peak sensitivity upwards.

Comparisons to CMDL Aircraft Observations



NOTE: We needed to adjust RTA transmittance tuning by a factor of 1.025 to achieve agreement with CMDL

Comparison of CH4 product & CMDL Continuous Ground Site



Barrow Alaska

3deg. x 3deg. gridded retrieval averaged over 60-70 lat, & -165 to -90 lng

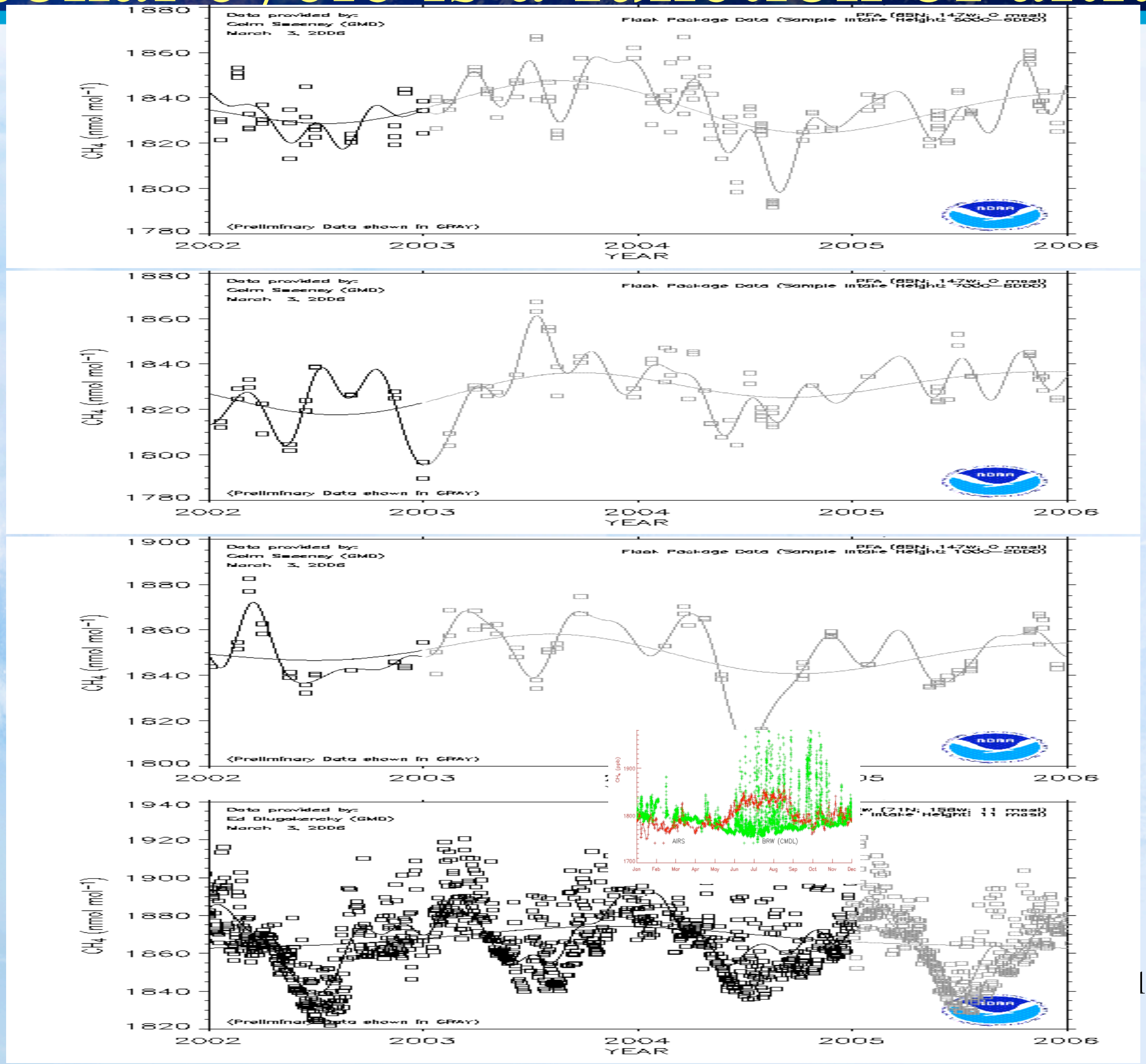
CMDL Poker Flats, Alaska
Seasonal cycle is a function of altitude

7.5 km
385 mb

5.5 km
500 mb

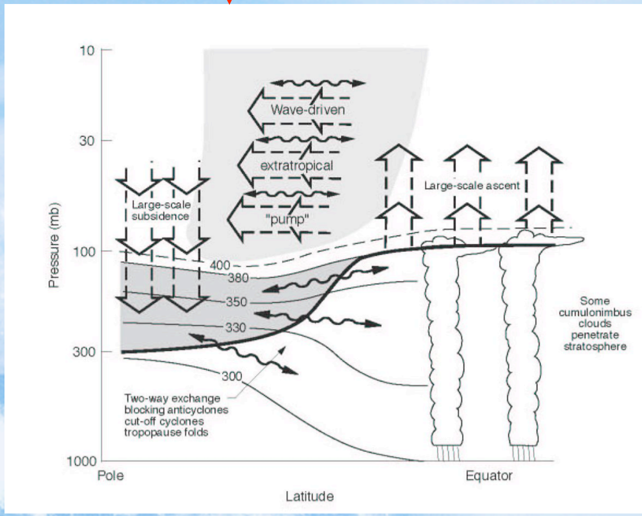
1.5 km
850 mb

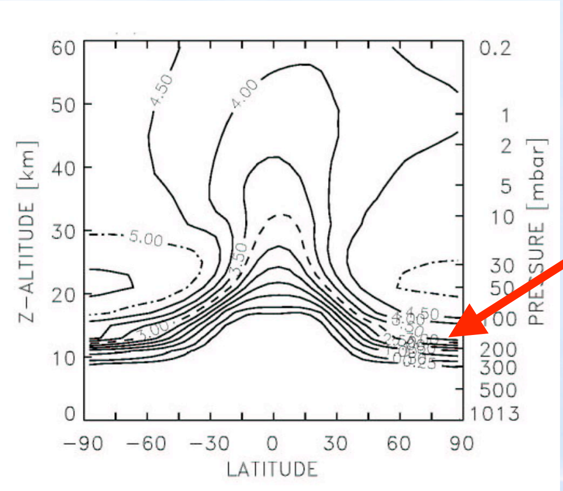
Surface
Flasks
(Barrow)



How much of our CH4 signal is from stratospheric air?

Dobson-Brewer circulation

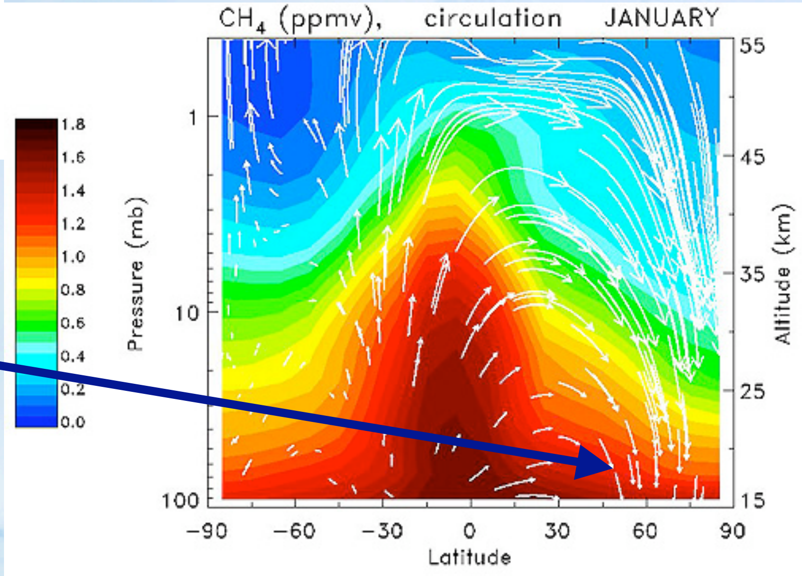




UT/LS region in high latitudes has "older" air.

We will explore tracer correlations to unravel surface vs stratospheric sources. (*working w/* L. Pan)

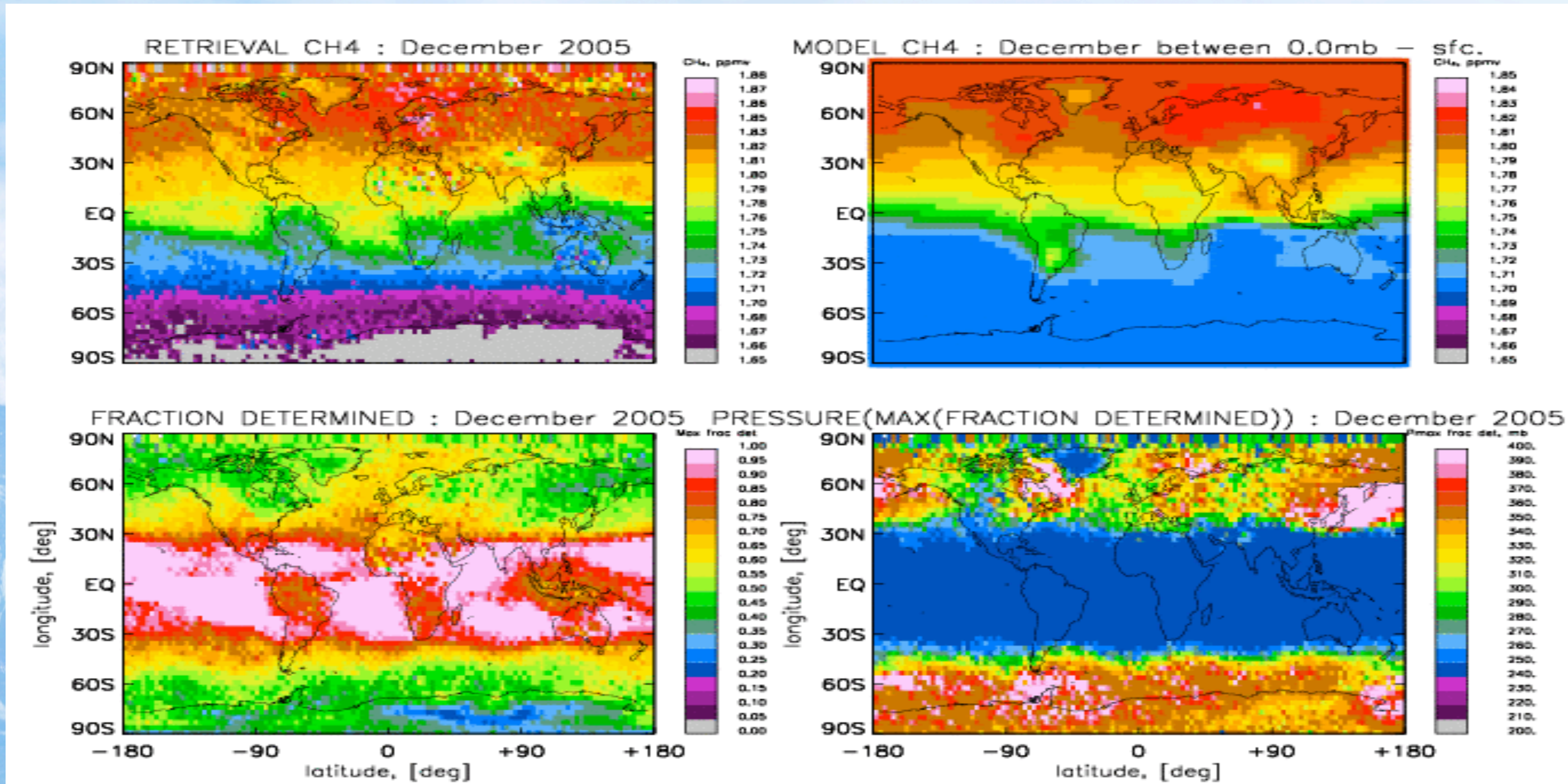
Can depress high latitude, high altitude methane signals in winter/spring time-frame.



Also providing the vertical information content to understand CH4 product

AIRS mid-trop measurement column

CH4 total column f/ transport model (Sander Houweling, SRON)



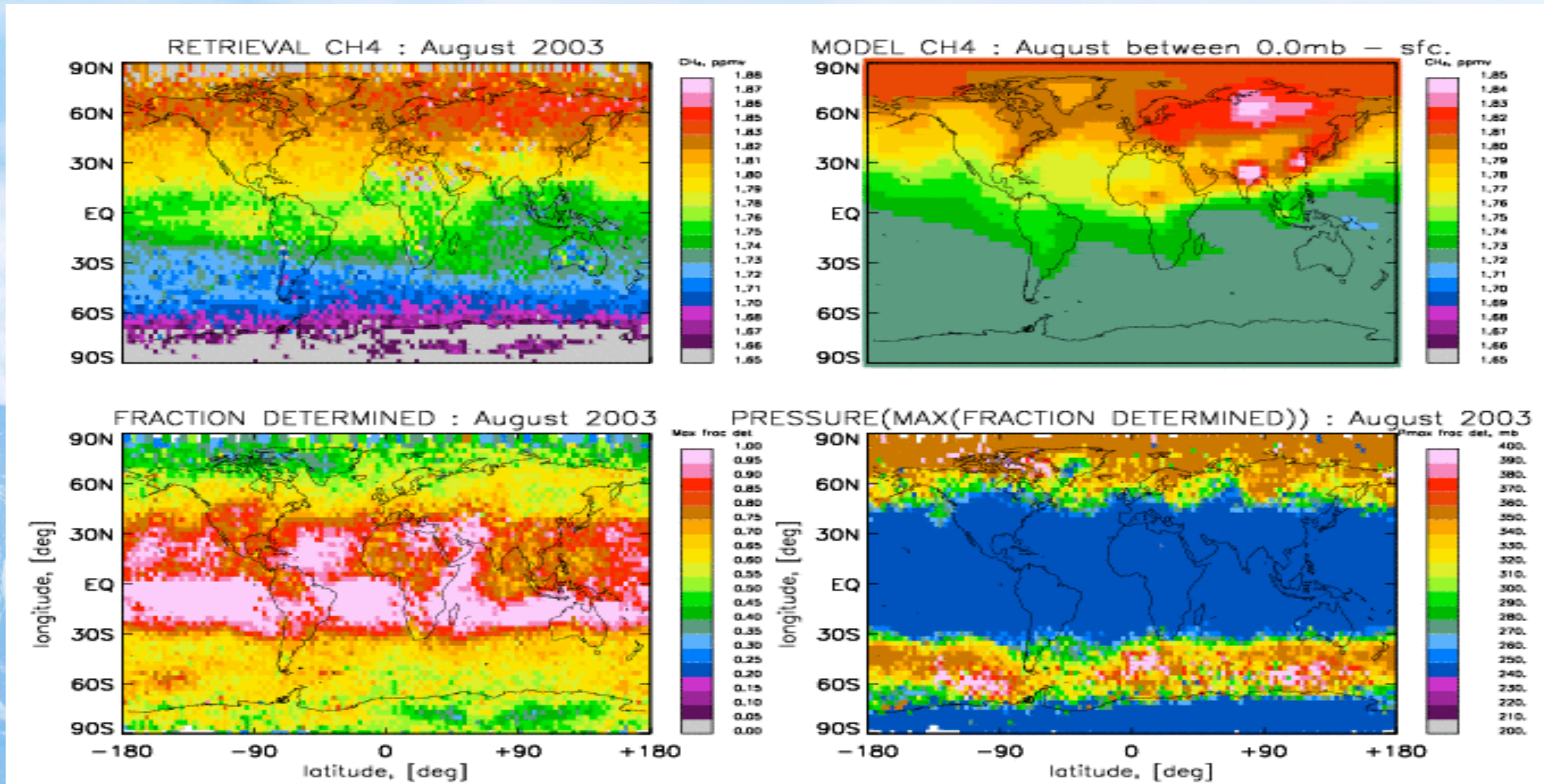
Fraction Determined from AIRS Radiances

Peak Pressure of AIRS Sensitivity

29 Months of AIRS Methane Product

AIRS mid-trop measurement column

CH4 total column f/ transport model (Sander Houweling, SRON)



Fraction Determined from AIRS Radiances

Peak Pressure of AIRS Sensitivity

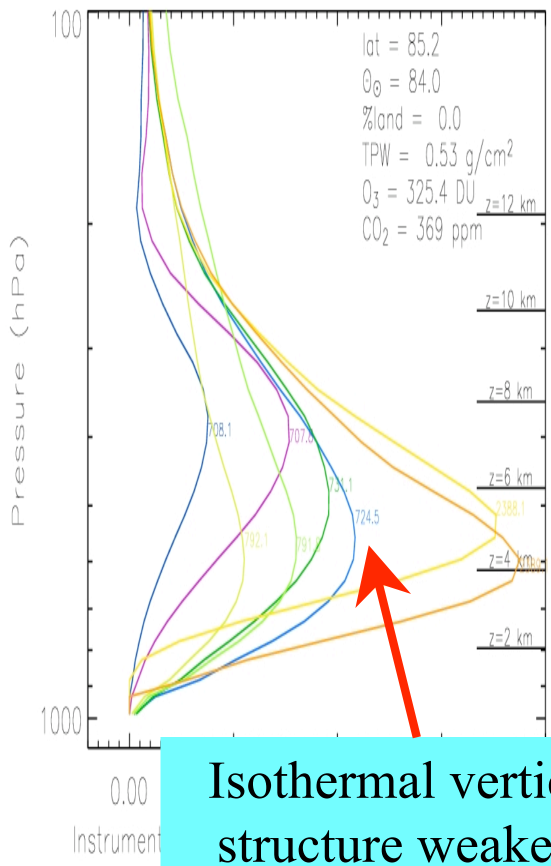
Carbon Dioxide and the Carbon Budget

- Lifetime in atmosphere is $\approx$ 100 years
  - conversion to limestone ($CaCO_2$) is main sink.
- +5.5 ± .3 GT-C/yr from fossil fuel emissions
  - A car emits 5 lbs of C per gallon, at 25 m/g that is a charcoal briquette every ¼ mile (Gerry Stokes)
- +1.6 ± .8 GT/yr from biomass burning
- Atmospheric concentration is well measured (Charles Keeling, Scripts) + 1.5 ppmv-CO2/yr = 3.3 ± .1 GT-C/yr
- Huge Terrestrial Annual Exchange (photosynthesis/respiration), 90 GT-C/yr
- Huge Ocean Exchange (phytoplanckton life cycle),
  - 90 GT-C/yr exchange
  - NET sink of -2.0 ± .2 GT-C/yr
- -1.8 ± 0.9 GT-C/yr unknown sink
  - Most like terrestrial or unknown ocean process.

LW Thermal CO_2 Kernel Functions are also Sensitive to H_2O, T(p), & O_3(p).

Polar

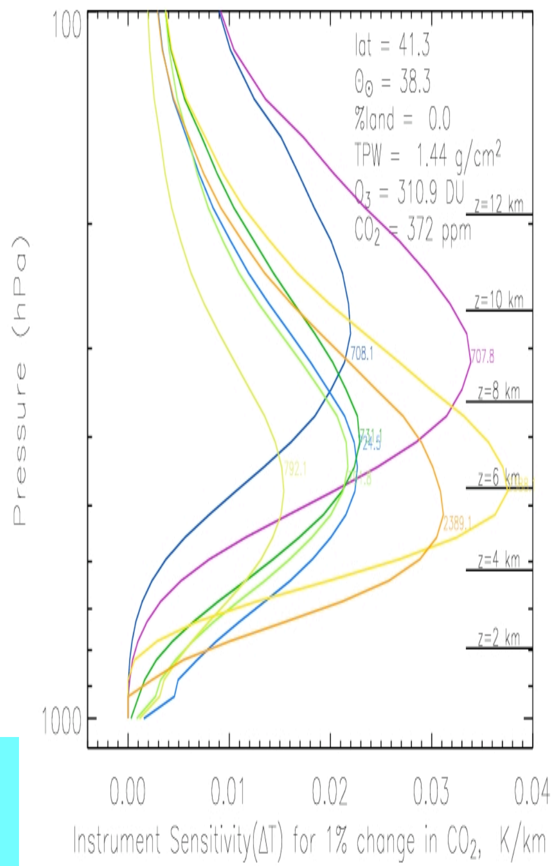
TPW = 0.5 cm



Isothermal vertical structure weakens sensitivity

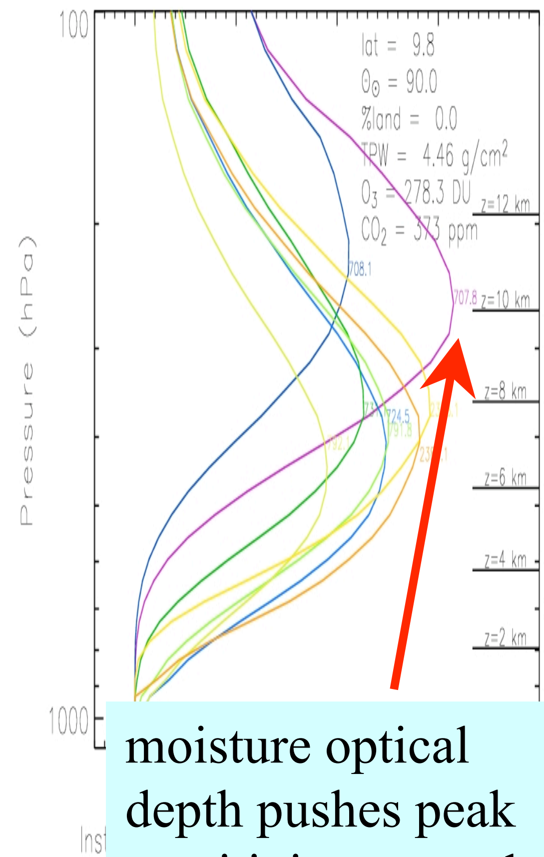
Mid-Latitude

TPW = 1.4 cm



Tropical

TPW = 2.5 cm



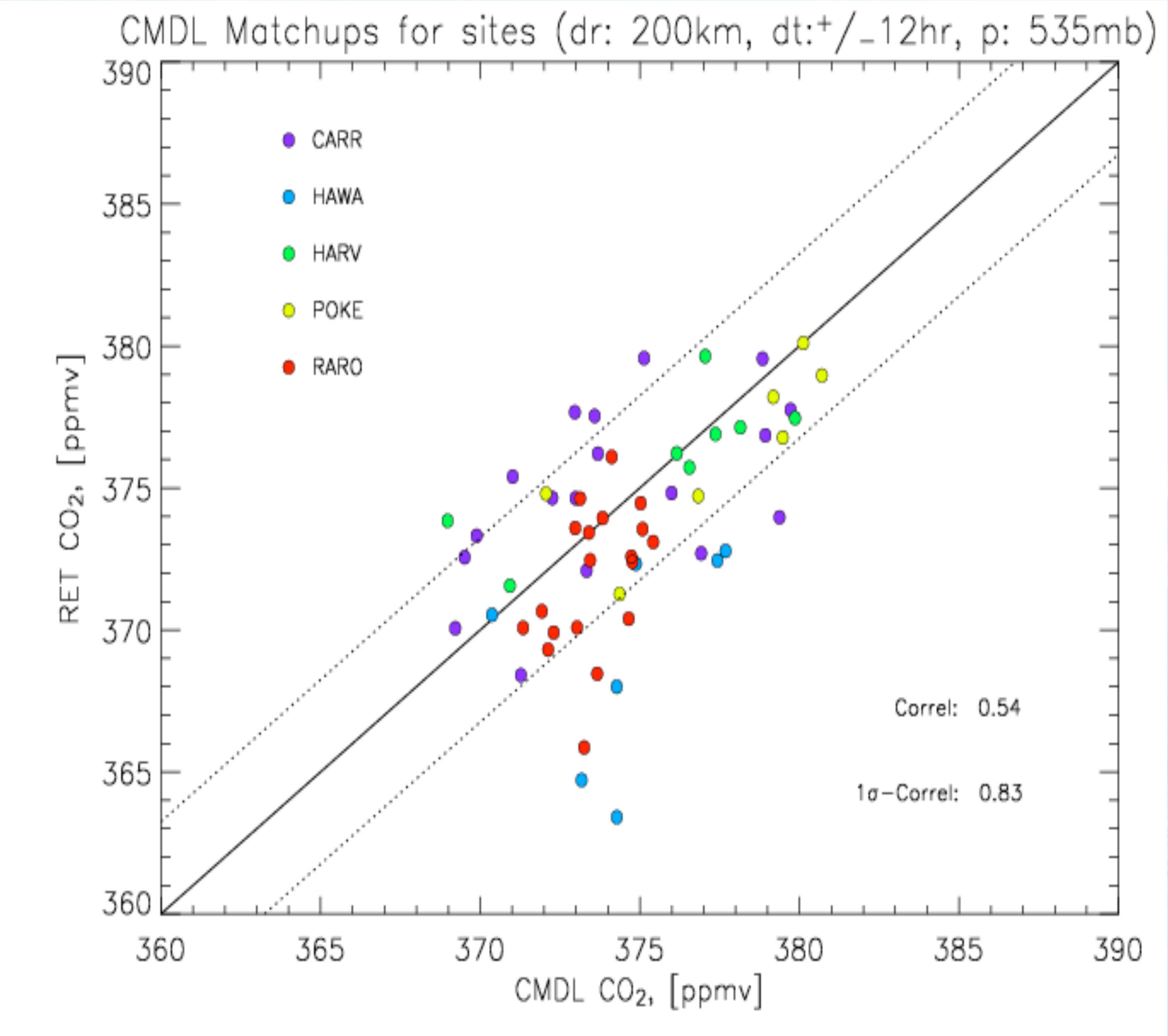
moisture optical depth pushes peak sensitivity upwards

Use of SW channels

- With recent improvements to RTA and tuning we can now use more SW information
- Care must be taken to separate temperature and CO_2 information in the minimization context.
  - Current algorithm uses SW for lower trop T(p) and LW for upper trop T(p) & CO2
  - Current algorithm does not utilize any model information for T(p), q(p), or O3(p), i.e., everything except surface pressure is derived from AMSU & AIRS radiances.
  - Microwave does not significantly impact T/CO2 separability due to high noise & side-lobe issues (*e.g.* AMSU-5 (500 mb) has 0.2 K NEDT, 2 K side-lobe correction.)
- We are looking into utilization of SW channels.

Preliminary Comparisons to CMDL aircraft

- AIRS “golf-balls” matched with CMDL.
  - Usually ≥ 5 hour time difference
  - Limit retrievals within 200 km
- Retrieval is average of “good” retrievals
  - 3 – 50 ret’s are used in each dot.
- Investigating outliers

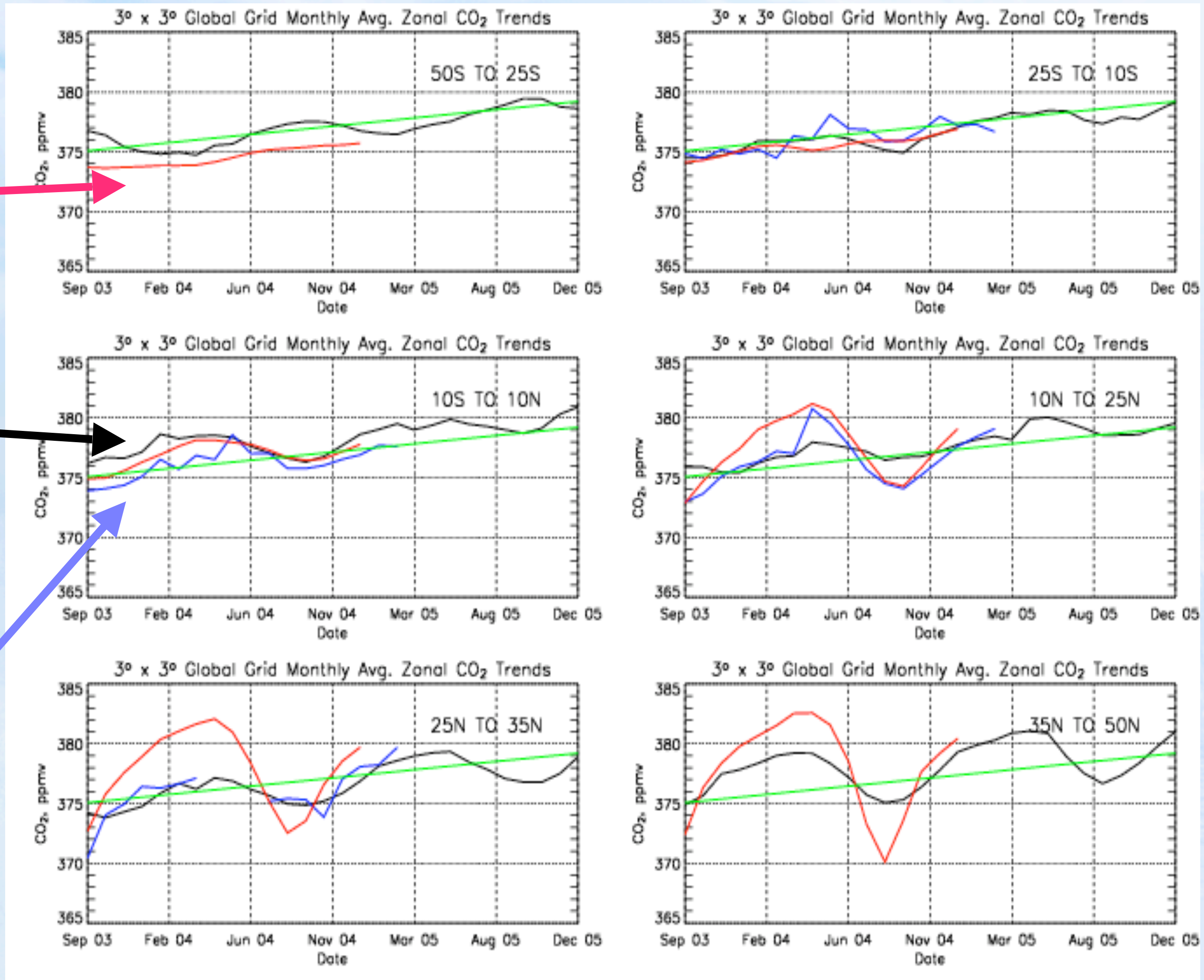


Comparisons to JAL aircraft observations & CMDL MDL model

CMDL Marine Boundary Layer Model

AIRS CO2 retrieval from GRIDDED dataset (sparse spatial sampling (we need to re-do this analysis w/ full spatial AIRS)

Matsueda *et al.* 2002 aircraft

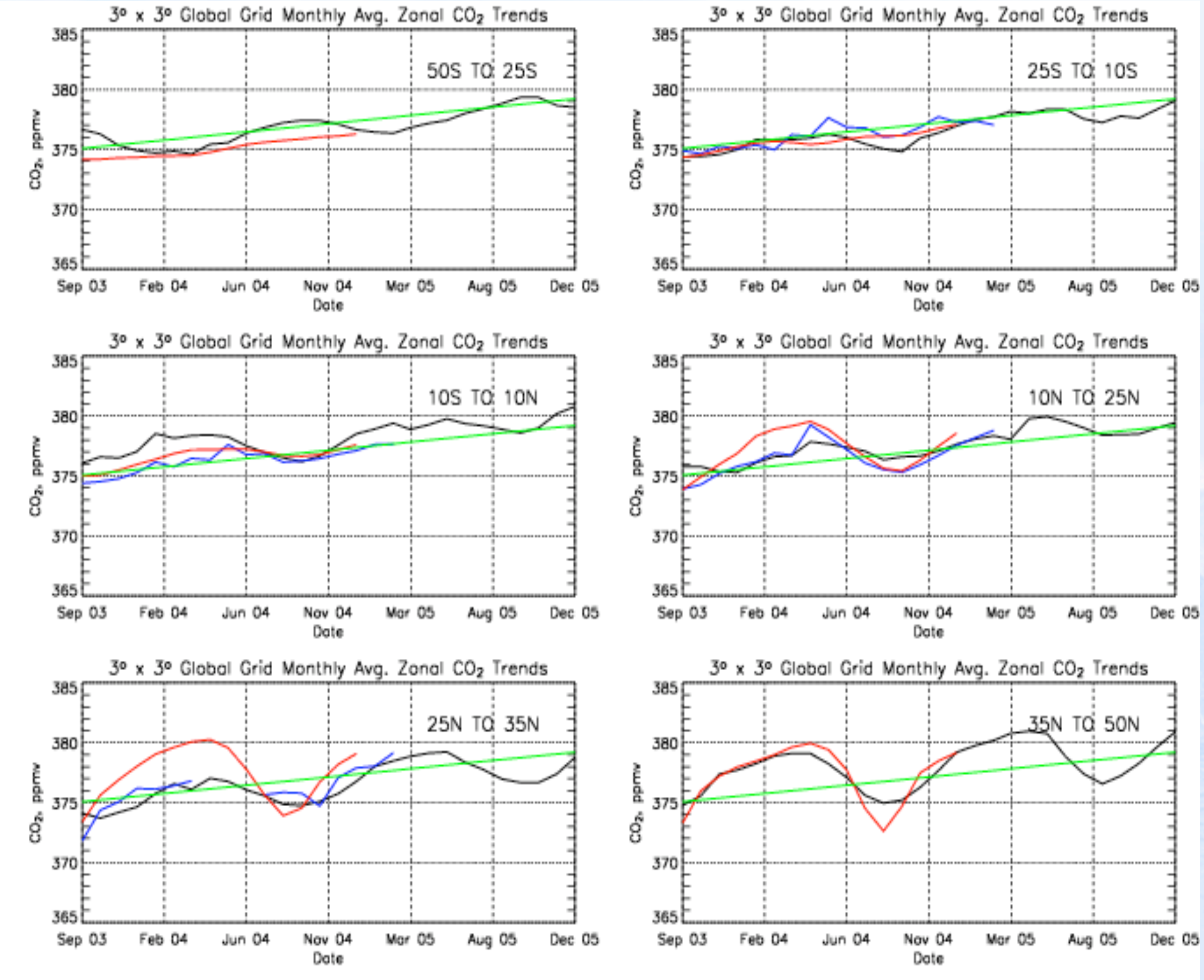


JAL Aircraft data provided by H. Matsueda

Same as before, but in-situ CO_2 adjusted by *a-priori* in retrieval

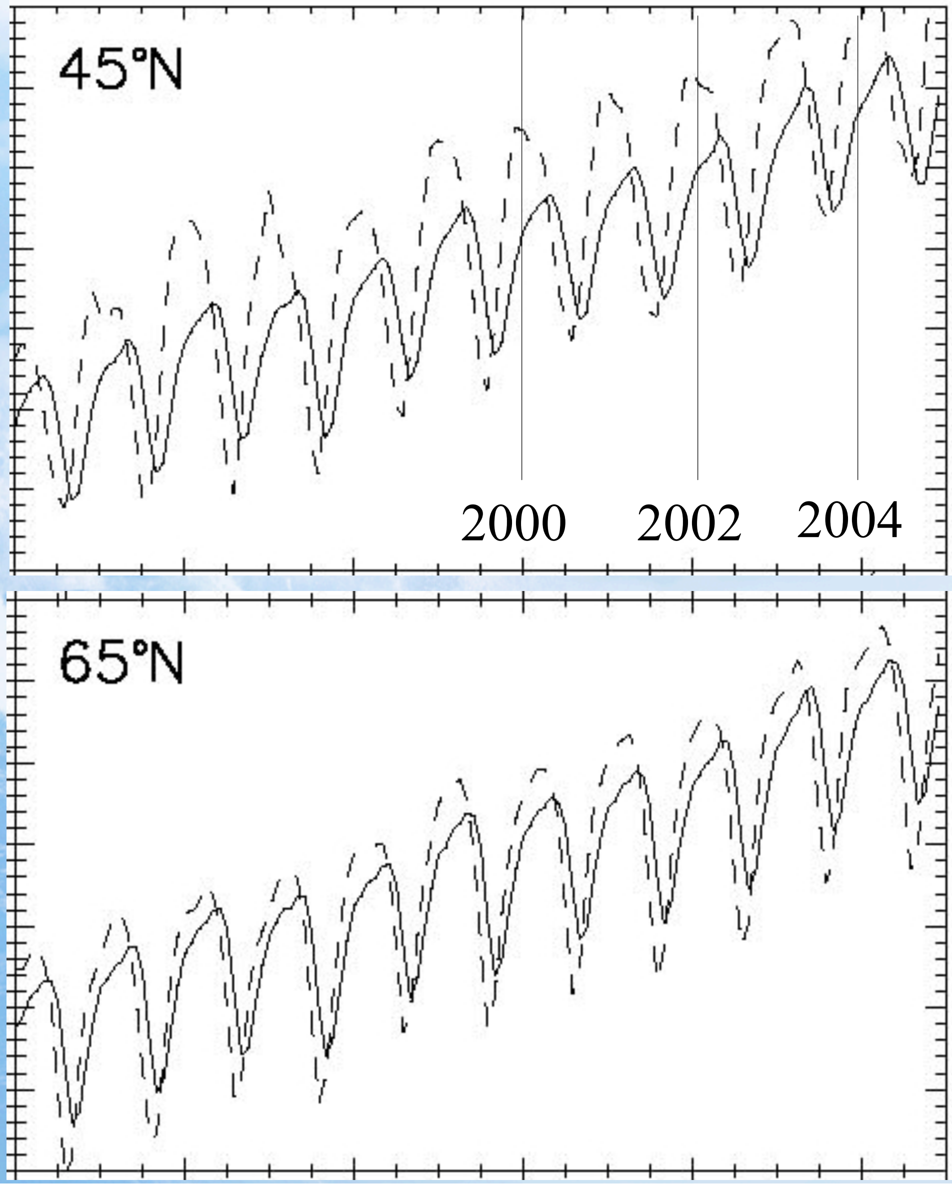
In-situ data is adjusted by the % of *a-priori* in our regularized retrieval. This depresses the seasonal amplitude of the *in-situ* data.

Differences should exist between single level (surface or altitude) observations and AIRS thick layer observations.



JAL Aircraft data provided by H. Matsueda

Again, to what extent does stratospheric age of air play a role?



Surface measurements (dashed line) and model of 500 mb concentration (solid line)

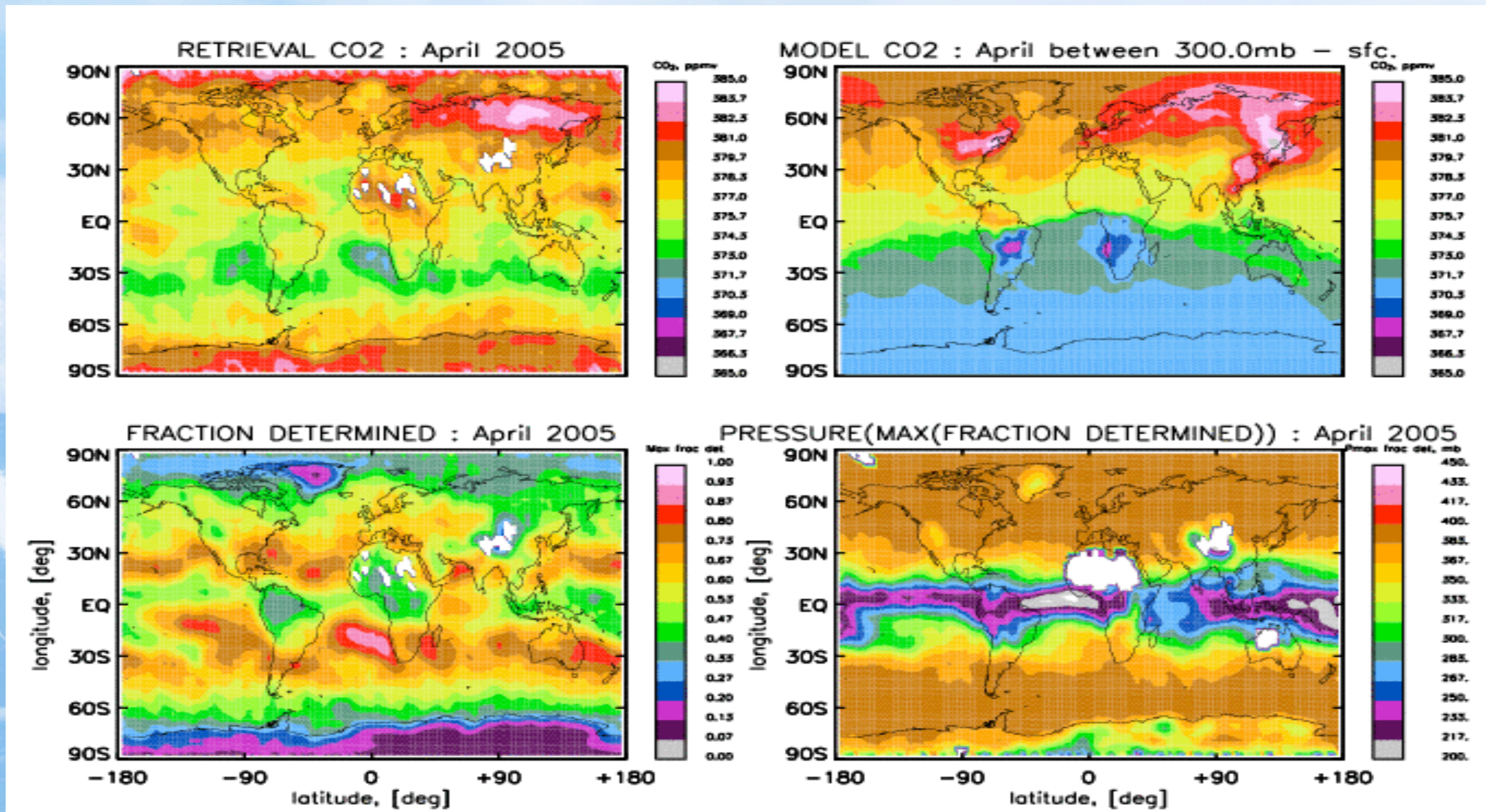
Brewer-Dobson effect has altitude, latitude, and seasonal variation with a maximum in northern winter.

Model runs of Brewer-Dobson circulation effect are courtesy of Run-Lie Shiaa, Mao-Chang Liang, Charles E. Miller, and Yuk L. Yung

Also providing the vertical information content & comparing CO_2 product with models

AIRS mid-trop measurement column

CO_2 Model Kawa (GSFC)



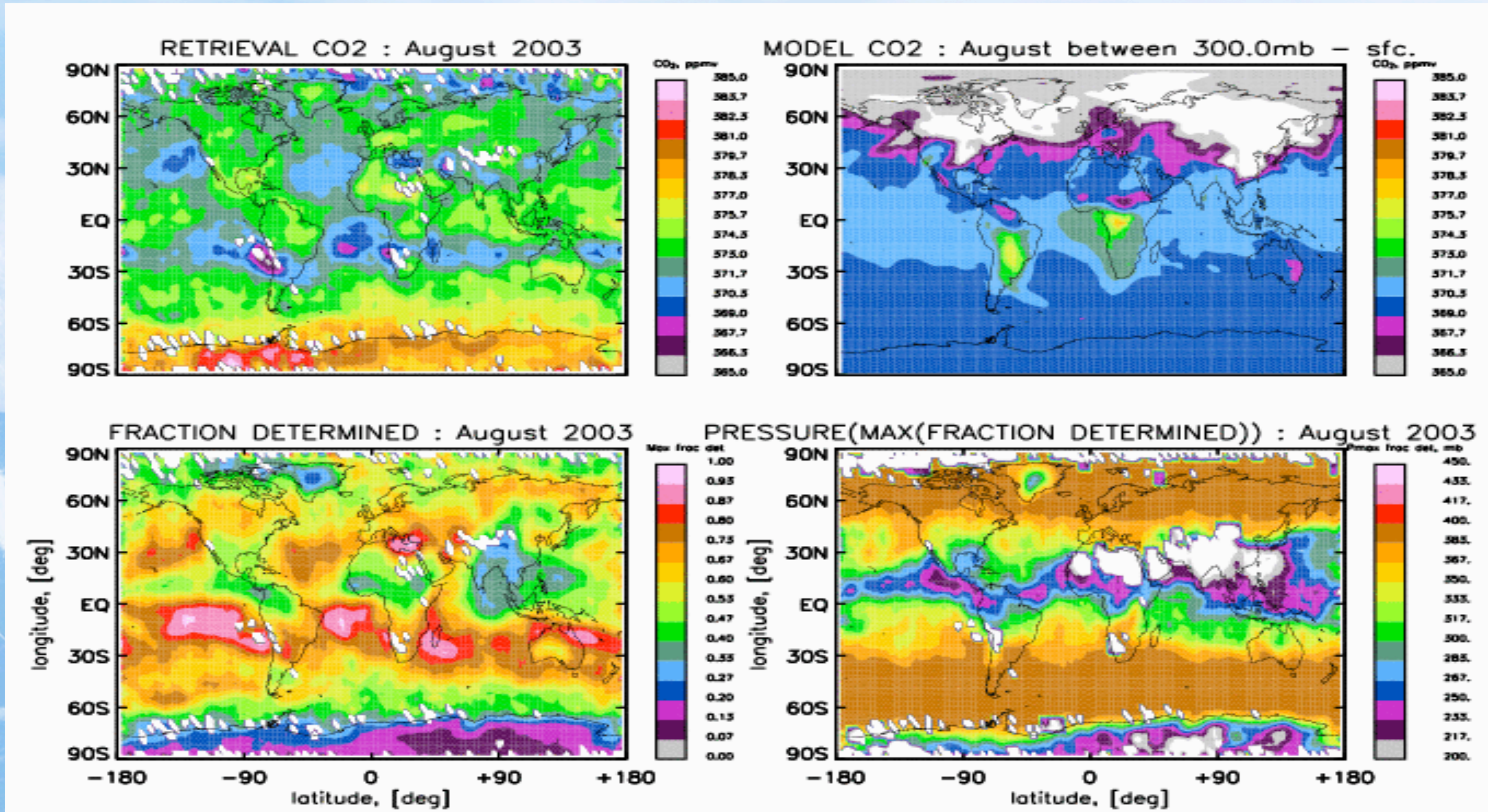
Fraction Determined from AIRS Radiances

Averaging Function Peak Pressure

29 Months of AIRS CO_2 Product

AIRS mid-trop measurement column

CO_2 Model Kawa (GSFC)



Fraction Determined from AIRS Radiances

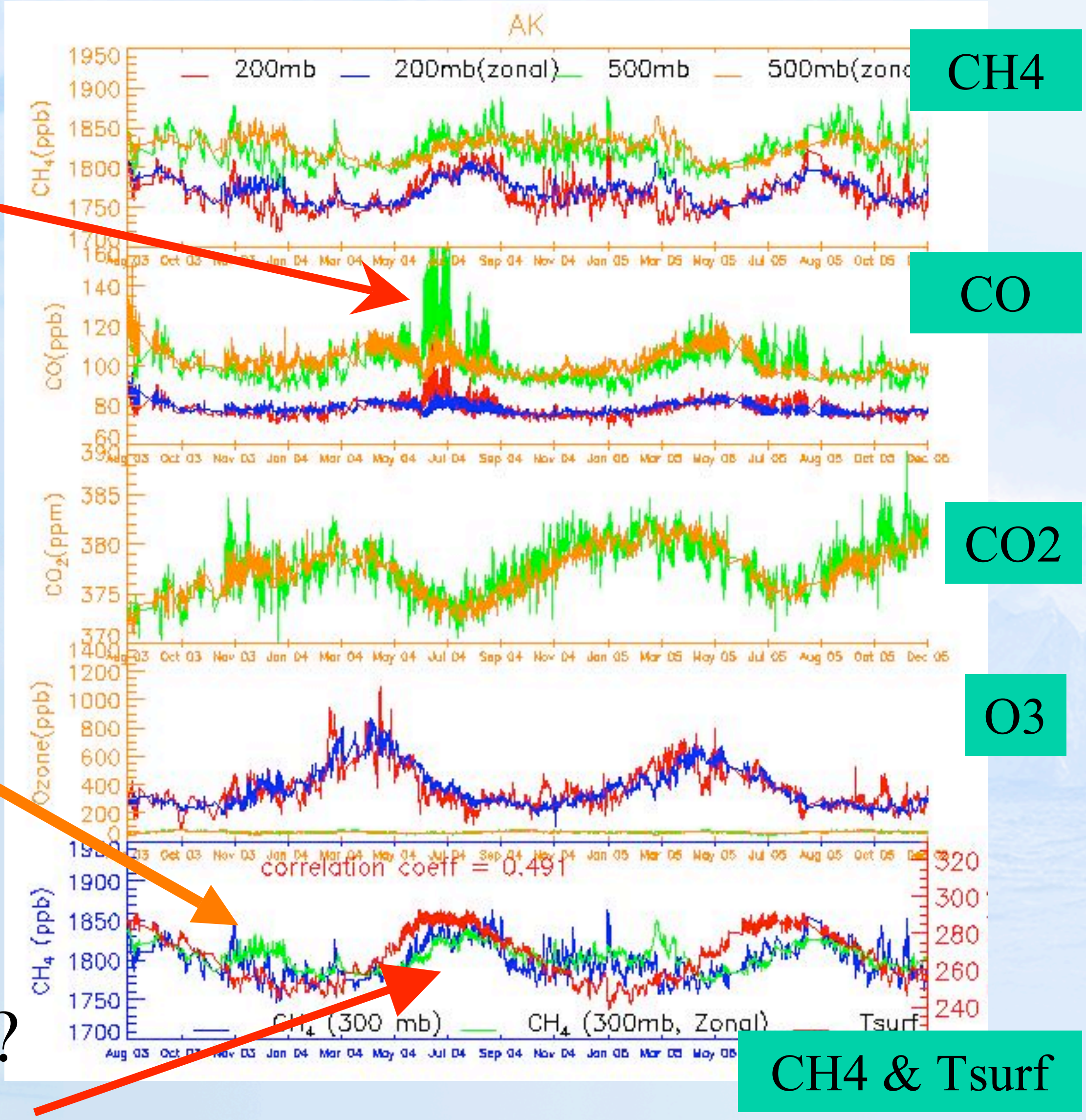
Averaging Function Peak Pressure

29 month time-series of AIRS products
Alaska & Canada Zone (60 ≤ lat ≤ 70, -165 ≤ lon ≤ -90)

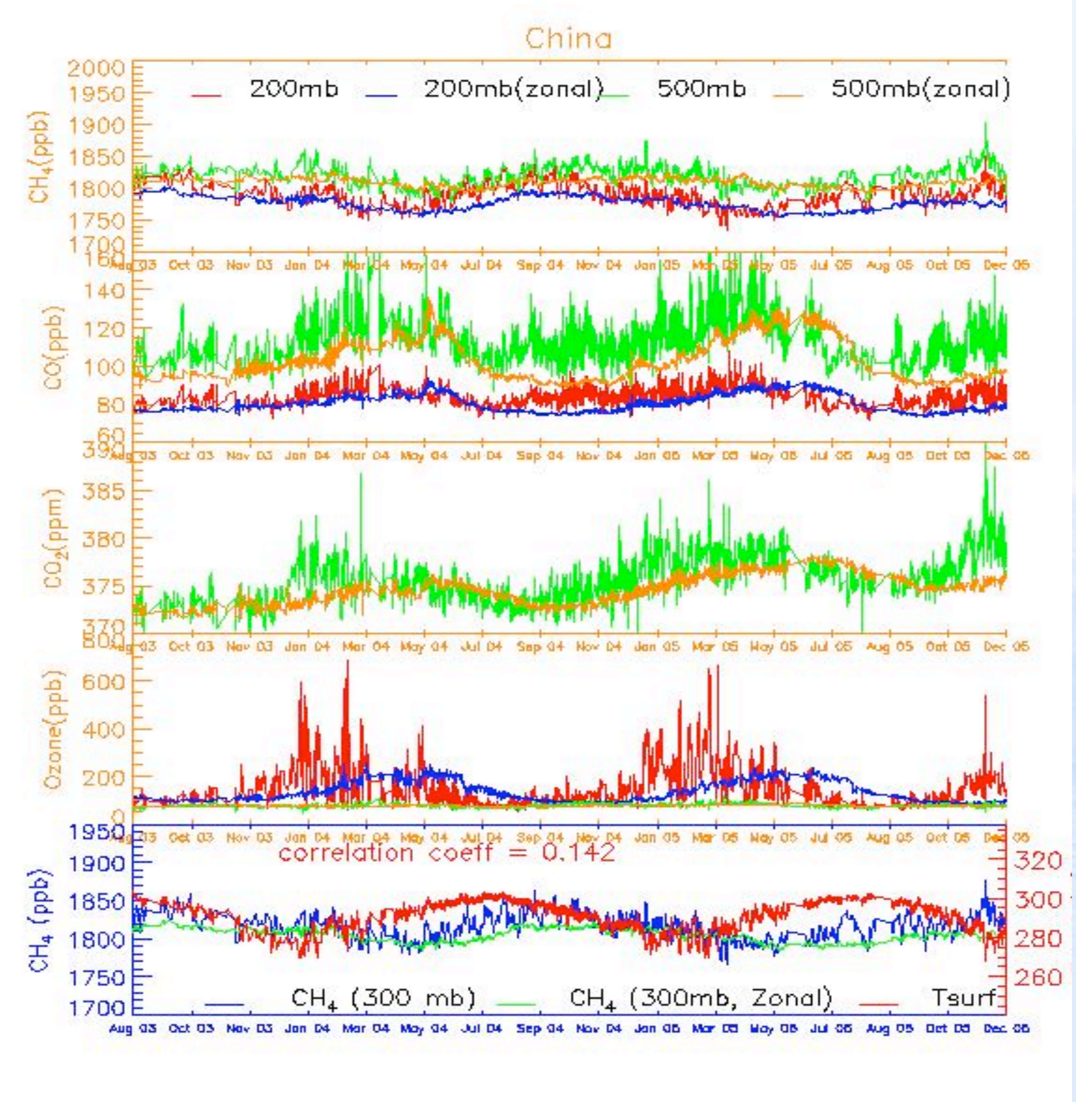
Fire (7/04)

??

Peat Wetlands?

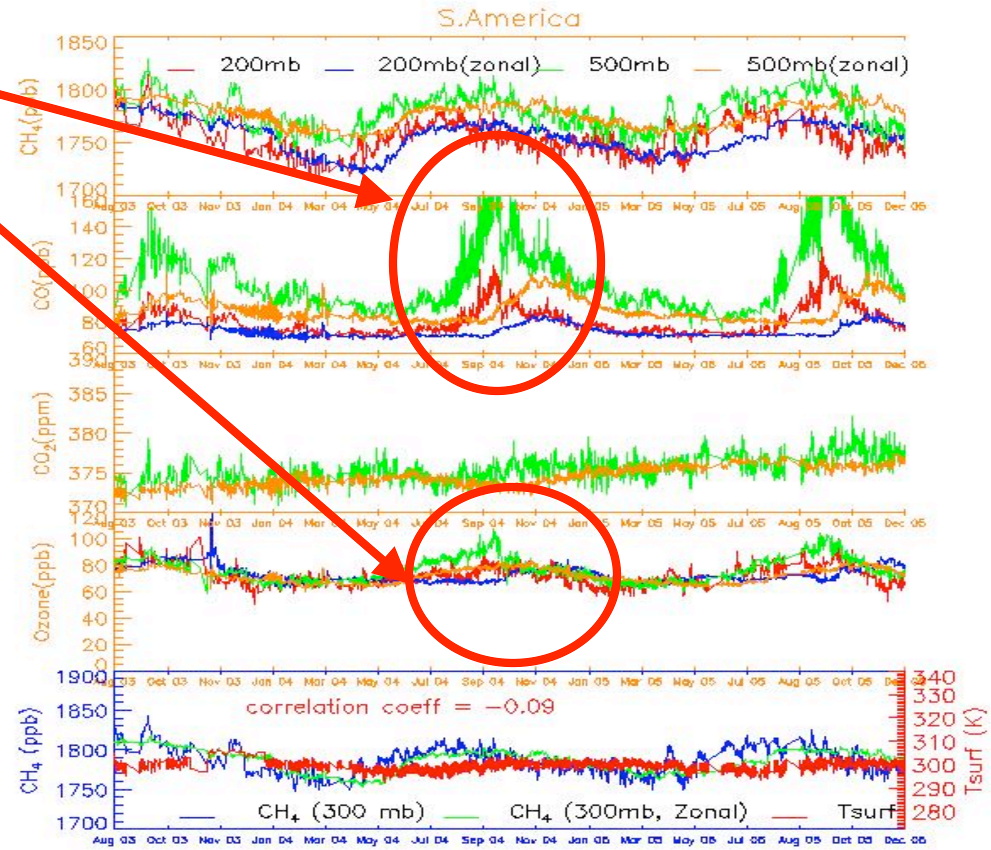


29 month time-series of AIRS products
Eastern China Zone (20 ≤ lat ≤ 45, 110 ≤ lon ≤ 130)



29 month time-series of AIRS products
South America Zone (-25 ≤ lat ≤ EQ , -70 ≤ lon ≤ -40)

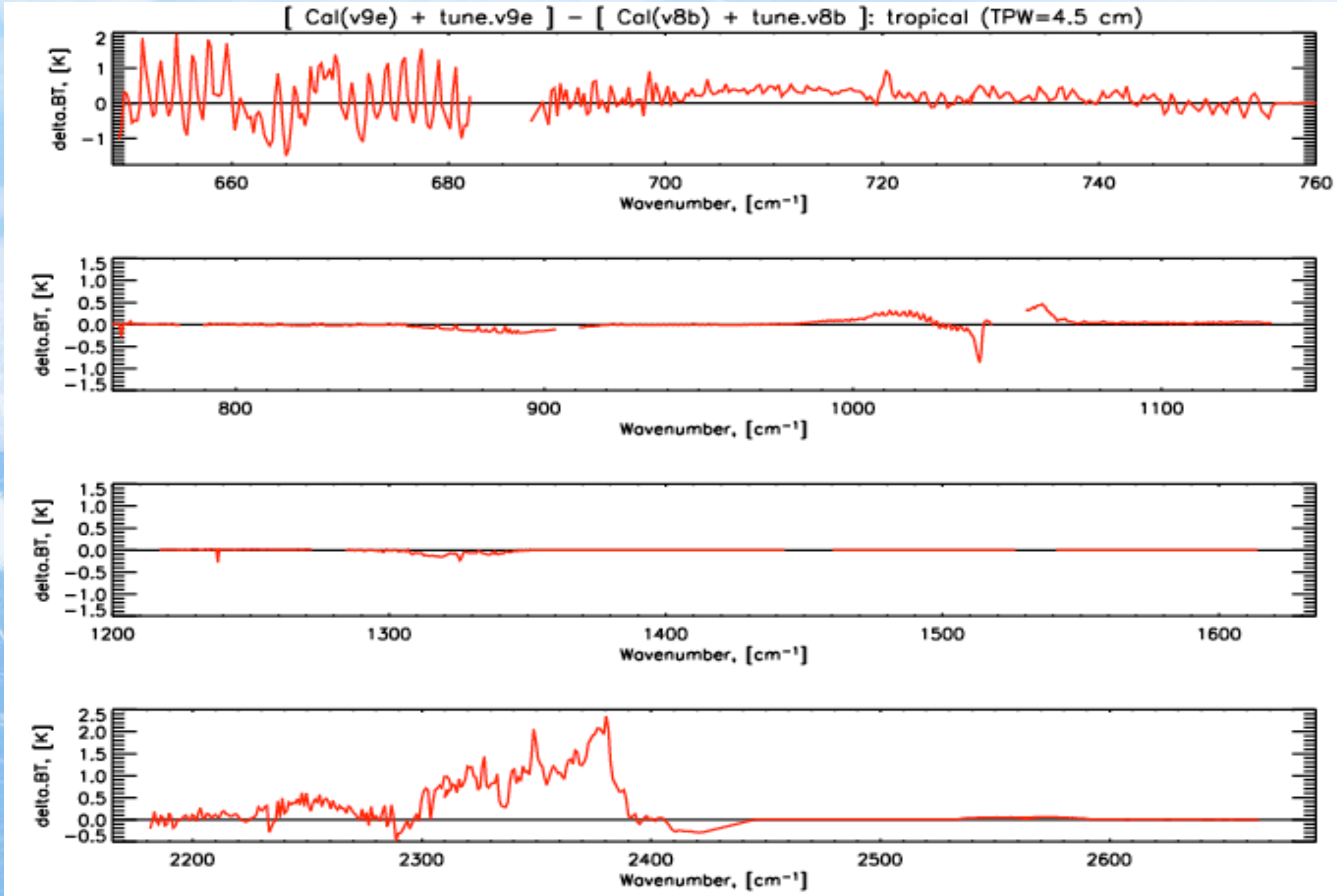
Biomass burning



NOAA AIRS CO2 Product is Still in Development

- Measuring a product to 0.5% is inherently difficult
  - Empirical bias correction (a.k.a. tuning) for AIRS is at the 1 K level and can affect the CO2 product.
  - Errors in moisture of ±10% is equivalent to ±0.7 ppmv errors in CO2.
  - Errors in surface pressure of ±5 mb induce ±1.8 ppmv errors in CO2.
  - AMSU side-lobe errors minimize the impact of the 57 GHZ O2 band as a T(p) reference point.
  - Bottom Line: *Core product retrieval must be flawless*.
- We can characterize seasonal and latitudinal mid-tropospheric variability.
- The real questions is whether thermal sounders can contribute to the source/sink questions.
  - Requires accurate vertical & horizontal transport models
  - Having simultaneous O_3, CO, CH_4, and CO_2 products is a unique contribution that thermal sounders can make.

Example: Radiance Differences between v8b (v4.0) and v9e (v5.0) RTA



NOAA/NESDIS Strategy: Use existing operational sounders.

Operational polar-orbiting instruments will provide global soundings in cloudy or clear conditions for the next 20+ years.

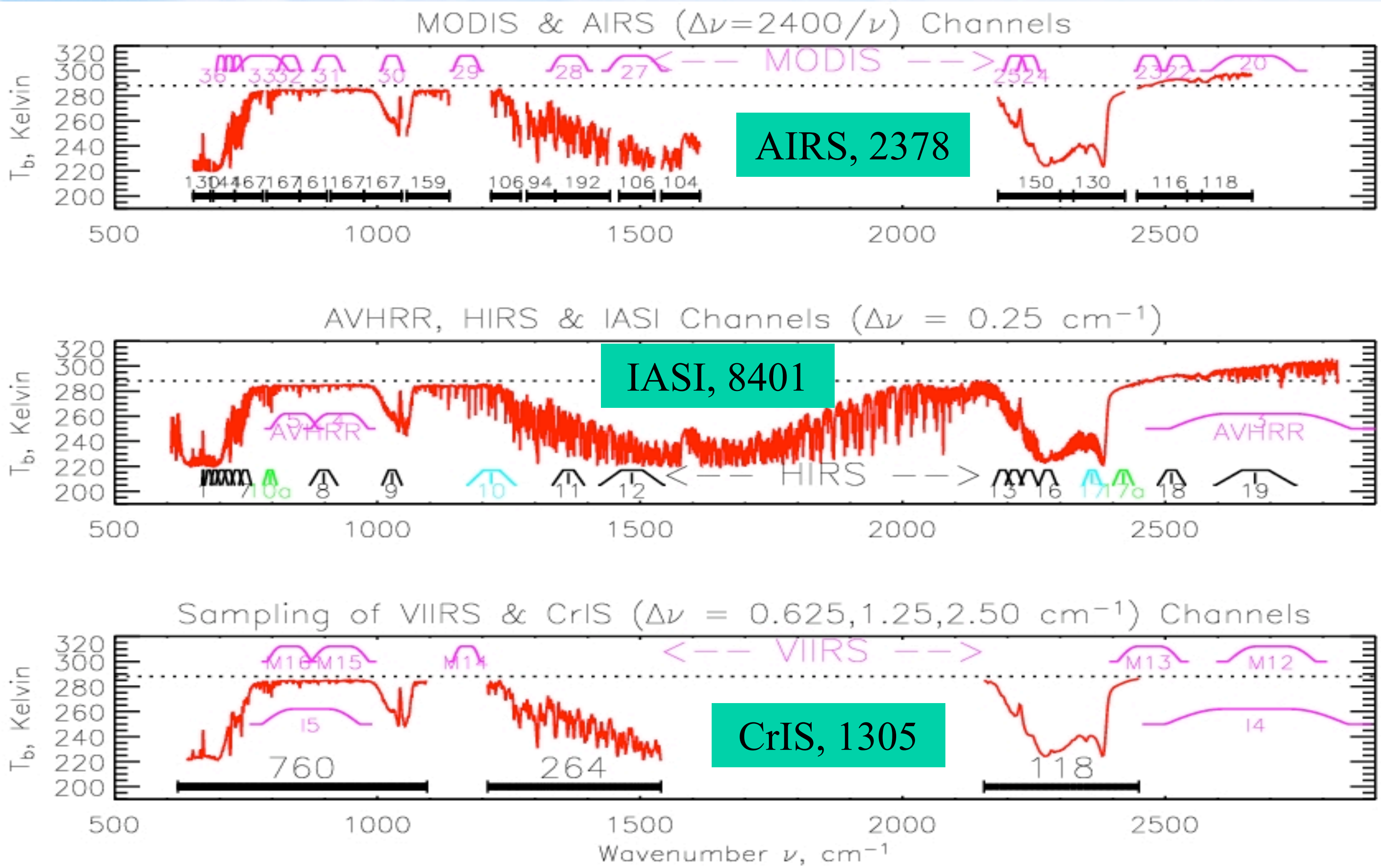
- Now: Develop core and test trace gas algorithms using the Aqua AIRS/AMSU/MODIS (May 4, 2002) Instruments
  - Compare products to *in-situ* (*e.g.*, CMDL Aircraft, JAL, INTEX, etc.) to characterize error characteristics.
  - The A-train complement of instruments (*e.g.*, MODIS, AMSR, Calipso) can be used to study effects of clouds, surface emissivity, etc.
- 2006: Migrate the AIRS/AMSU/MODIS algorithm into operations with METOP/IASI/AVHRR (2006,2011,2016)
  - Study the differences between instruments, *e.g.*, effects of scene and clouds on IASI's instrument line-shape.
- 2008: Migrate the AIRS/IASI algorithm into operations for NPP (2008) & NPOESS (2012,2015) CrIS/ATMS/VIIRS. These are part of the "NOAA Unique Products" within the NOAA NPOESS Data Exploitation (NDE) program.
- 2012: Migrate AIRS/IASI/CrIS algorithm into GOES-R/HES/ABI

Trace Gas Product Potential from Operational Thermal Sounders

gas	Range (cm^{-1})	Precision	Interference	
O_3	1025-1050	10%	H2O,emissivity	Working
CO	2080-2200	15%	H2O,N2O	
CH_4	1250-1370	20 ppb	H2O,HNO3	
CO_2	680-795 2375-2395	2 ppm 2 ppm	H2O,O3	
SO_2	1340-1380	1000%	H2O,HNO3	In Work
HNO_3	860-920 1320-1330	40% 25%	emissivity H2O,CH4	
N_2O	1250-1315 2180-2250	10% 10%	H2O H2O,CO	
$CFCl_3$ (F11)	830-860	20%	emissivity	Held Fixed
CF_2Cl (F12)	900-940	20%	emissivity	
CCl_4	790-805	50%	emissivity	

Haskins, R.D. and L.D. Kaplan 1993

Spectral Coverage of AIRS, IASI, and CrIS



Will Continue our Investigation of Algorithms

- We recently ran a system in which zeroes and infinite components of our regularization were removed.
  - Makes SVD approach equivalent to linear constrained regularization.
  - Results are indistinguishable from current PGE approach.
  - However, Vertical Averaging Functions (VAF) are more robust.

$$\boldsymbol{X}_j^i = \boldsymbol{X}_j^A + \left[\boldsymbol{K}_{j,n}^T \cdot \boldsymbol{N}_{n,n}^{-1} \cdot \boldsymbol{K}_{n,j} + \boldsymbol{C}_{j,j}^{-1}\right]^{-1} \cdot \boldsymbol{K}_{j,n}^T \cdot \boldsymbol{N}_{n,n}^{-1} \cdot \left[\boldsymbol{R}_n^{obs} - \boldsymbol{R}_n(\boldsymbol{X}^{i-1}) + \boldsymbol{K}_{n,j} \cdot \left(\boldsymbol{X}_j^{i-1} - \boldsymbol{X}_j^A\right)\right]$$

- Experiments with optimal estimation form (Equation above) of minimization.
  - PGE iterative form prohibits accurate assessment of VAF's.
  - Regression as *a-priori* & first guess (O_3) reduces accuracy of VAF's.
  - Use of MIT (for T,q) or climatology/model (O_3,CO,CH_4,CO_2) state as a-priori may reduce outliers due to cloud contamination and/or regression (T,q,O3,ε) interaction with the PGE iterative cloud clearing approach.
- Investigate the use of *a-priori* state and statistics in regularization
  - PGE methodology doesn't utilize statistical relationships (*a-priori* covariance information). What *a-priori* to use is the big issue.
  - Again, this *may* help to eliminate outliers and make VAF's more robust.

Conclusions and Summary

- High spectral resolution operational thermal sounders have the capability of measuring mid-tropospheric concentrations of atmospheric trace gases globally for the next 20+ years.
- CO product is robust and validation experiments are underway (*e.g.*, INTEX, W. McMillan, UMBC)
- CH_4 is more difficult: preliminary analysis appears promising but we need to understand stratospheric vs. surface contributions.
- CO_2 is significantly more difficult and many algorithms are being inter-compared. Re-processing of acquired AIRS (30 months, so far) & IASI radiances to optimize algorithm(s) will continue.
- AIRS, IASI, and CrIS may contribute to source/sink determination by simultanously measuring T(p), q(p), O_3(p), CO, CH_4, & CO_2 globally. One impact will be to provide upper air estimate for OCO.
- Working closely w/ CMDL to acquire more aircraft observations
- Other gas products (SO_2, HNO_3, N_2O) are in-work (thanks to Larrabee for incorporating these into the AIRS physics).